

Motivation

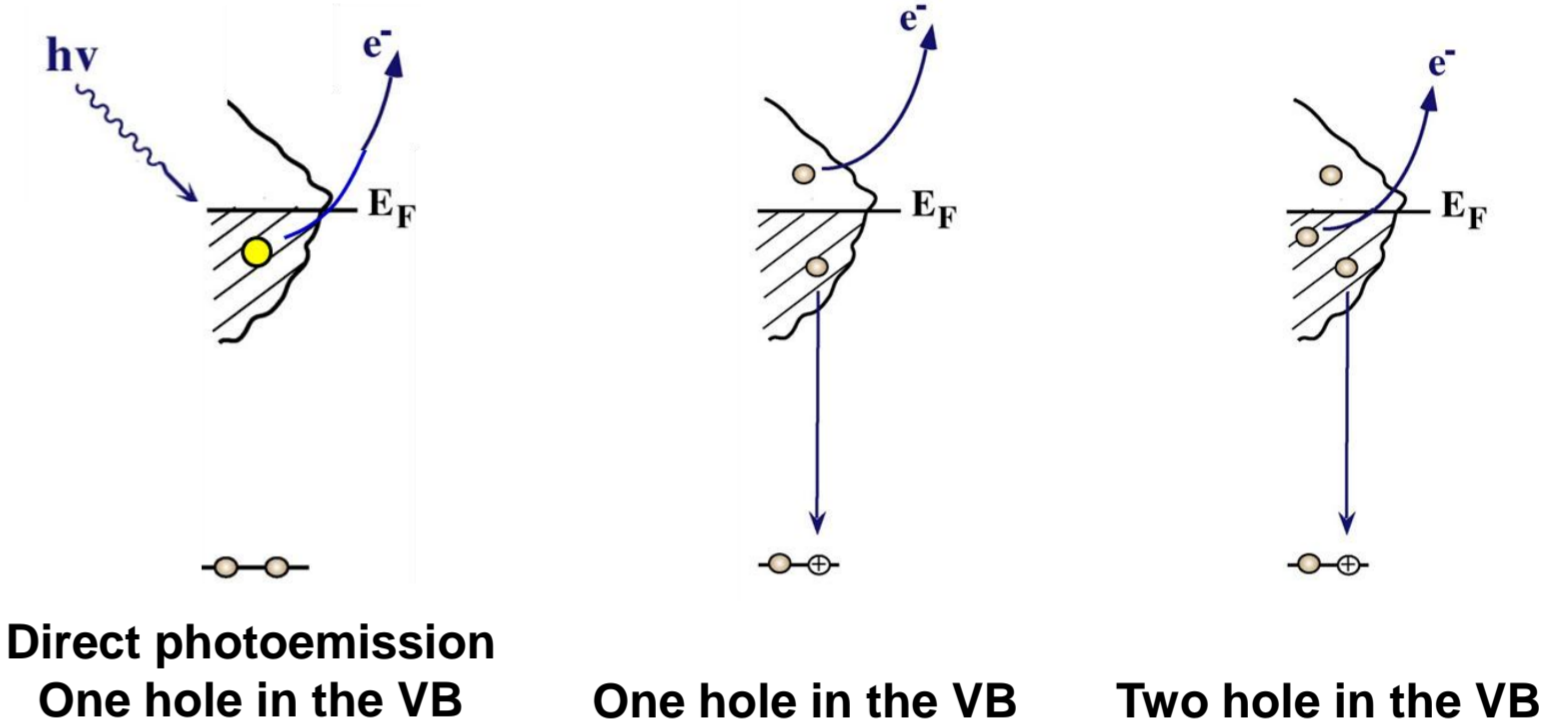
The semiconductor BiTeCl is attractive as a material exhibiting the large Rashba splitting of both the bulk and the surface states together with the large band gap. In addition to the fundamental interest, such materials could be useful for building spintronic devices. The core levels and band structure of Cl- and Te-terminated BiTeCl have been well investigated by x-ray (XPS) and angle-resolved (ARPES) photoemission spectroscopy [1, 2]. We decided to extend the experimental study of the electronic structure of this material by examine its reaction to changes in the excitation energy. For this purpose, resonant x-ray photoemission spectroscopy (ResPES) with the use of synchrotron radiation was chosen. This method allows distinguishing the contributions of the various components to the valence band (VB) and establishment of the regularities of formation of the electronic structure.

The BiTeCl crystal was grown based on BiCl₃-Bi₂Te₃ using a modified Bridgman method [3] and XRD verified for phase purity.

ResPES spectroscopy

Photoemission (PE) from the VB can be direct or two-stage [4]. In the first case, a valence electron directly absorbs a photon, leaves the sample. One hole remains in the final state. In the second case the photon is absorbed at core level and an excited state is observed: electron above the E_F and a hole at the core level. This state can decay through:

- **Elastic channel.** The electron can return to its place, then the released energy is transferred to a valence electron via an Auger process. This scenario leads to the same final state as the direct PE and gives an enhancement of the VB spectrum at the resonant energy.
- **Inelastic channel.** A valence electron can fill the core hole and a second valence electron is ejected from the sample. The final state now contains two holes in the VB and the electron above the E_F. This appears as an inelastic loss in the PE spectrum.

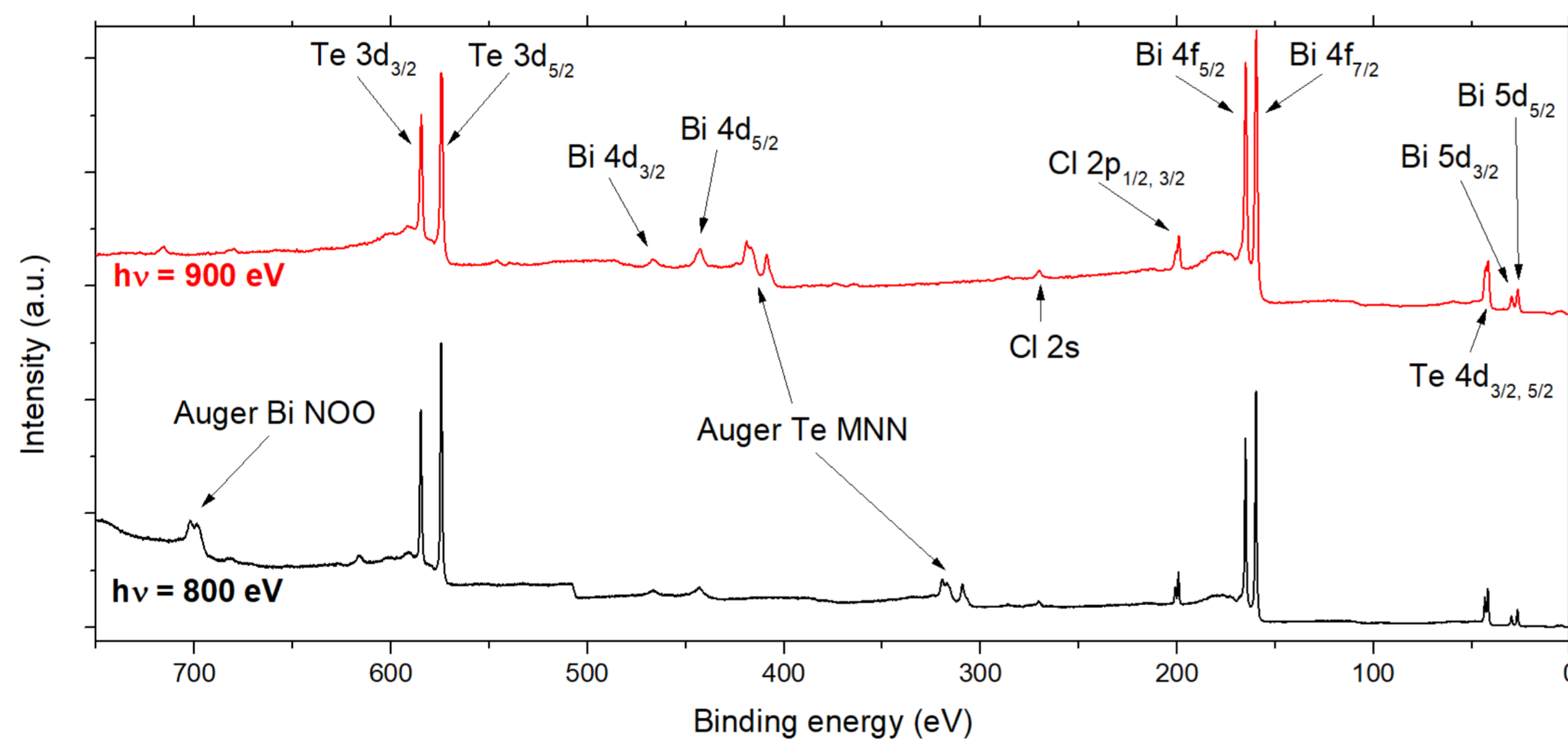


ResPES measurement by tuning the photon energy to an appropriate absorption threshold allows distinguishing the contributions of the various components to the occupied valence states. In addition to information on single-particle states, such experiments give the characteristics of strongly correlated two-hole and long-lived excited states.

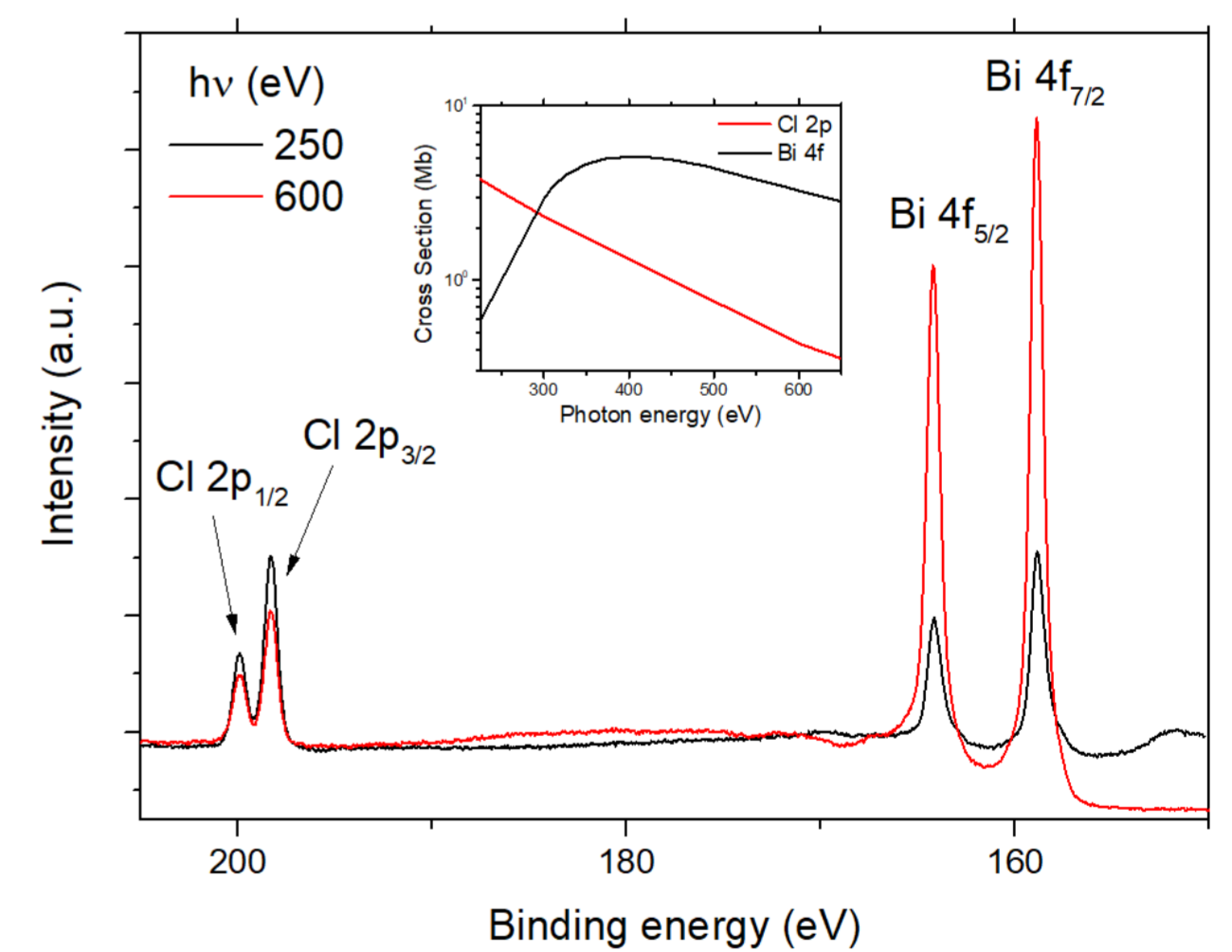
As continuous variation of the photon energy is mandatory for this method it can only be performed at synchrotron radiation facilities. All presented measurements were performed at the Russian-German laboratory of the BESSY II synchrotron (Berlin).

Results

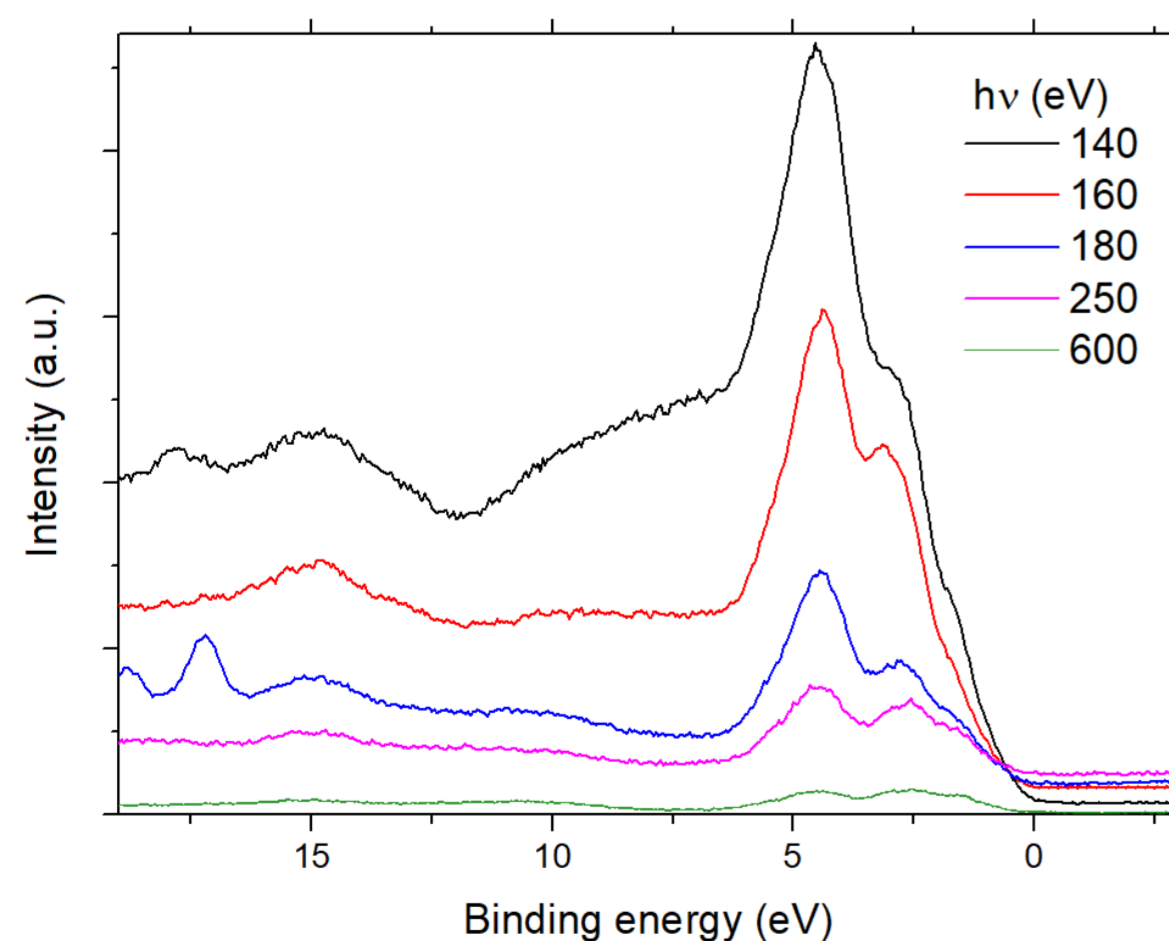
PE spectra of BiTeCl measured with photon energies $h\nu = 800$ and 900 eV.



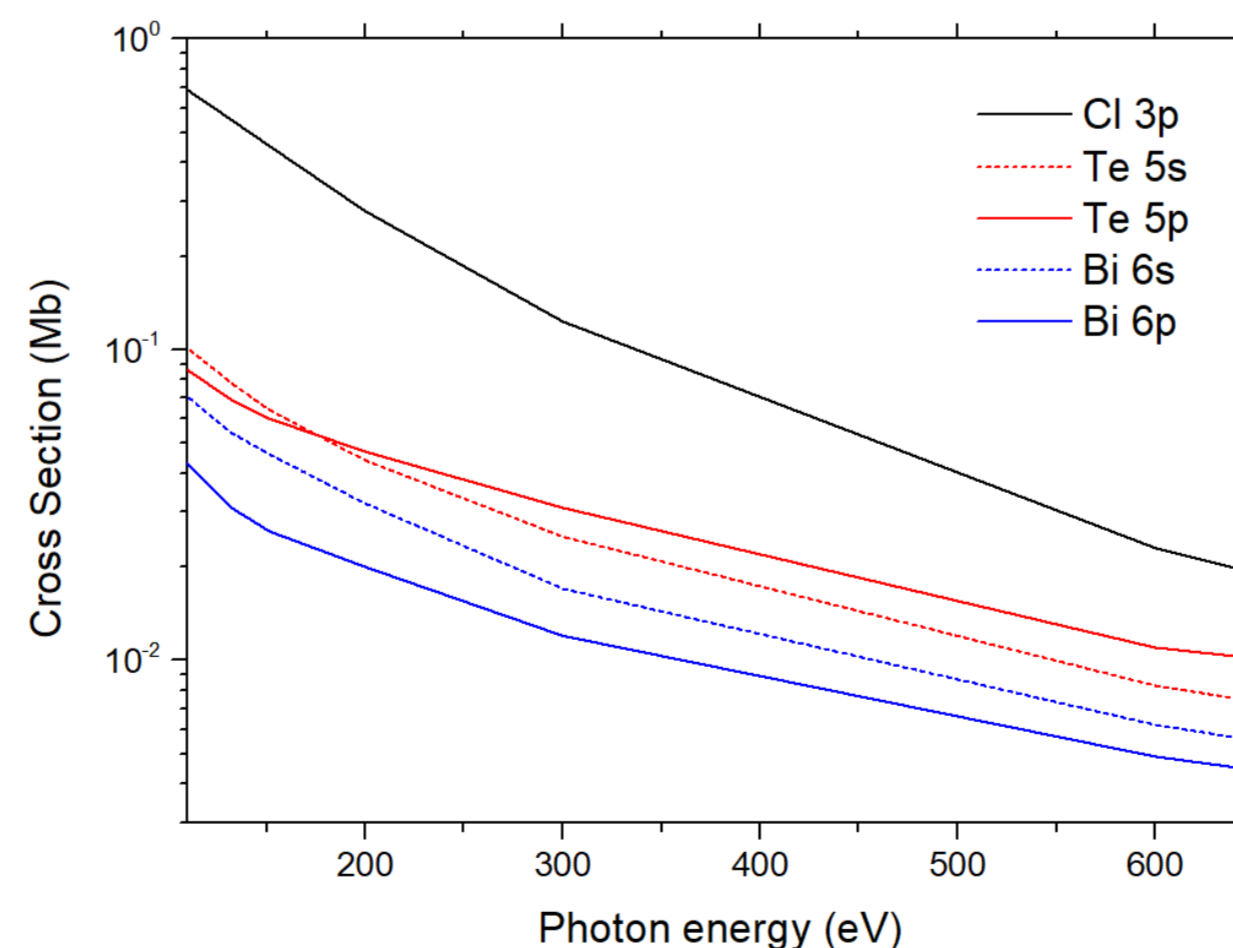
Bi 4f and Cl 2p core levels PE spectra of BiTeCl measured with $h\nu = 250$ and 600 eV. Insert shows the PE cross-sections [5] of these levels depending on $h\nu$.



VB PE spectra of BiTeCl at different $h\nu$ from 140 to 600 eV.



The PE cross-sections [5] for the same energy range.



- Tuning $h\nu$ through the absorption edges of Bi, Te and Cl levels did not cause changes in the VB spectra, meaning no resonance was observed.

- An enhancement of the intensity for the entire VB with $h\nu$ change from 600 to 140 eV. Two main bands centered at the binding energies 3 and 4.5 eV, the latter of which reveals a stronger enhancement.

- The PE cross-sections of the external levels change in a similar way, except Cl 3p cross-section, whose growth with $h\nu$ decrease is the fastest. → The band at 4.5 eV is mainly formed by the Cl 3p states, which is consistent with the calculated data [6]. The band at 3 eV is assigned mainly to the Te 5p states in accordance with [6].

References

1. L. Moreschini, et al., J. Electron Spectros. Relat. Phenomena. (2005) <https://doi.org/10.1016/j.elspec.2014.11.004>.
2. G. Landolt, et al., New J. Phys. 15 (2013) 085022.
3. K. A. Kokh, et al., J. Cryst. Growth 275 (2005) e2129.
4. T.V. Kuznetsova, et al., Bulletin of the Russian Academy of Sciences. Physics. 77(2) (2013) 226.
5. J.-J. Yeh and I. Lindau, At. Data Nucl. Data Tables 32 (1985) 1.
6. S. Zhou, et al., Mater. Sci. Semicond. Process. 27 (2014) 605.

Acknowledgements

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